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NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	DEC 01	ChemPort single article sales feature unavailable
NEWS 3	APR 03	CAS coverage of exemplified prophetic substances enhanced
NEWS 4	APR 07	STN is raising the limits on saved answers
NEWS 5	APR 24	CA/CAplus now has more comprehensive patent assignee information
NEWS 6	APR 26	USPATFULL and USPAT2 enhanced with patent assignment/reassignment information
NEWS 7	APR 28	CAS patent authority coverage expanded
NEWS 8	APR 28	ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS 9	APR 28	Limits doubled for structure searching in CAS REGISTRY
NEWS 10	MAY 08	STN Express, Version 8.4, now available
NEWS 11	MAY 11	STN on the Web enhanced
NEWS 12	MAY 11	BEILSTEIN substance information now available on STN Easy
NEWS 13	MAY 14	DGENE, PCTGEN and USGENE enhanced with increased limits for exact sequence match searches and introduction of free HIT display format
NEWS 14	MAY 15	INPADOCDB and INPAFAMDB enhanced with Chinese legal status data
NEWS 15	MAY 28	CAS databases on STN enhanced with NANO super role in records back to 1992
NEWS 16	JUN 01	CAS REGISTRY Source of Registration (SR) searching enhanced on STN
NEWS 17	JUN 26	NUTRACEUT and PHARMAML no longer updated
NEWS 18	JUN 29	IMSCOPROFILE now reloaded monthly
NEWS 19	JUN 29	EPFULL adds SLART to AB, MCLM, and TI fields
NEWS EXPRESS	MAY 26	09 CURRENT WINDOWS VERSION IS V8.4, AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.
NEWS HOURS		STN Operating Hours Plus Help Desk Availability
NEWS LOGIN		Welcome Banner and News Items

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:34:53 ON 30 JUN 2009

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 15:35:04 ON 30 JUN 2009
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 JUN 2009 HIGHEST RN 1160357-19-6
DICTIONARY FILE UPDATES: 29 JUN 2009 HIGHEST RN 1160357-19-6

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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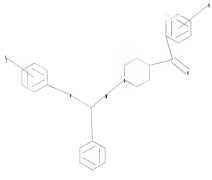
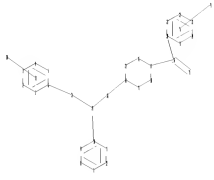
Uploading C:\Program Files\Stnexp\Queries\10594105carbonyl.str





chain nodes :
25 26 27 30 34 36 37
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24
chain bonds :
6-25 10-27 14-26 17-36 20-36 25-27 26-27 36-37
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24
exact/norm bonds :
6-25 13-14 13-18 14-15 14-26 15-16 16-17 17-18 25-27 26-27 36-37
exact bonds :
10-27 17-36 20-36
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24
20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

G1:C,N

G2:CF2,CF3,CC12,CC13,CBr2,CBr3,X

G3:C,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 30:CLASS
31:Atom 34:CLASS 35:Atom 36:CLASS 37:CLASS

L1 STRUCTURE UPLOADED

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:35:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 685 TO ITERATE

100.0% PROCESSED 685 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

L2 6 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 185.88 186.10

FILE 'CAPLUS' ENTERED AT 15:35:33 ON 30 JUN 2009
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FILE COVERS 1907 - 30 Jun 2009 VOL 151 ISS 1
FILE LAST UPDATED: 29 Jun 2009 (20090629/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

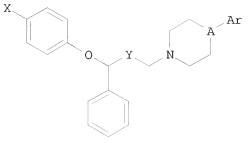
=> s l2 full
L3 2 L2

=> d ibib abs hitstr tot
THE ESTIMATED COST FOR THIS REQUEST IS 11.28 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

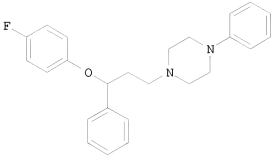
L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1103625 CAPLUS
DOCUMENT NUMBER: 143:387060
TITLE: Preparation of piperazine or piperidine derivatives as serotonin reuptake inhibitors
INVENTOR(S): Pinney, Kevin G.; Miranda, Maria Graciela; Dorsey, James Michael
PATENT ASSIGNEE(S): Baylor University, USA
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005094896	A2	20051013	WO 2005-US10356	20050328
WO 2005094896	A3	20070503		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AP, EA, EP, OA				
EP 1732610	A2	20061220	EP 2005-730778	20050328
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
US 20080132514	A1	20080605	US 2007-594105	20070921
PRIORITY APPLN. INFO.:			US 2004-557069P P	20040326
			WO 2005-US10356 W	20050328

OTHER SOURCE(S): CASREACT 143:387060; MARPAT 143:387060
GI



I



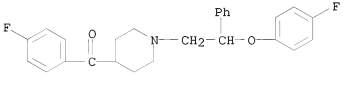
II

AB Title compds. I [X = F or CF3; Y = (CH2)n; n = 0-1; A = N or C; Ar = aryl] and their pharmaceutically acceptable salts, are prepared and disclosed as serotonin reuptake inhibitors. Thus, e.g., II was prepared by reduction of 1-phenyl-3-(4-phenyl-piperazin-1-yl)-propan-1-ol (preparation given) using sodium borohydride followed by coupling with 4-fluorophenol. The ability of I to inhibit [3H]5-HT uptake was evaluated using liquid scintillation spectroscopy and it was revealed that selected compds. of the invention possessed IC50 values in the range of 1.45 up to 9.56 μM. I as serotonin reuptake inhibitors should prove useful in the treatment of depression. Pharmaceutical composition comprising I are disclosed.

IT 866548-42-7P 866548-43-8P 866548-44-9P
866548-45-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperazine or piperidine derivs. as serotonin reuptake inhibitors)

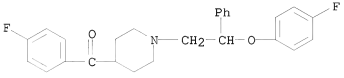
RN 866548-42-7 CAPLUS

CN Methanone, [1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-piperidinyl](4-fluorophenyl)- (CA INDEX NAME)

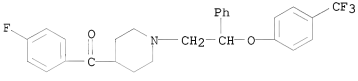


RN 866548-43-8 CAPLUS

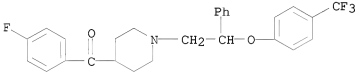
CN Methanone, [1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-piperidinyl](4-fluorophenyl)-, hydrochloride (1:1) (CA INDEX NAME)



RN 866548-44-9 CAPLUS
CN Methanone, (4-fluorophenyl)[1-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-4-piperidinyl]- (CA INDEX NAME)



RN 866548-45-0 CAPLUS
CN Methanone, (4-fluorophenyl)[1-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-4-piperidinyl]-, hydrochloride (1:1) (CA INDEX NAME)



L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2003:860624 CAPLUS
DOCUMENT NUMBER: 140:76994

TITLE: Syntheses and Binding Studies of New [(Aryl)(aryloxy)methyl]piperidine Derivatives and Related Compounds as Potential Antidepressant Drugs with High Affinity for Serotonin (5-HT) and Norepinephrine (NE) Transporters

AUTHOR(S): Orjales, Aurelio; Mosquera, Ramon; Toledo, Antonio; Pumar, M. Carmen; Garcia, Neftali; Cortizo, Lourdes; Labeaga, Luis; Innerarity, Ana

CORPORATE SOURCE: Research Department, FAES FARMA S. A., Leioa, Vizcaya, 48940, Spain

SOURCE: Journal of Medicinal Chemistry (2003), 46(25), 5512-5532
CODEN: JMCMAR; ISSN: 0022-2623

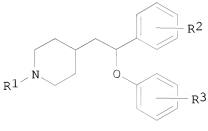
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:76994

GI



I

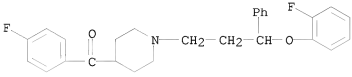
AB In a wide search program toward new, efficient, and fast-acting antidepressant drugs, series of new compds. having an (aryl)(aryloxy)methyl moiety linked directly or through a methylene chain to different substituted and unsubstituted cycles (isoquinoline, piperazine, piperidine, tetrahydropyran, or cyclopentane) were prepared These compds. have been evaluated for their affinities for serotonin (5-HT) transporter (SERT) and 5-HT1A and 5-HT2A receptors. Racemic mixts. of 4-[(aryl)(aryloxy)methyl]piperidines I (R1 = H, Me, MeCO; R2 = H, 3-F, 4-F, 4-Cl, 4-Me; R3 = H, 2-CN, 4-O2N, 4-MeO, 2-Ph, etc.) showed much higher affinity values for SERT than fluoxetine and resulted in lack of affinity for 5-HT1A and 5-HT2A receptors. Some of these racemic mixts. were resolved to their enantiomers and tested for binding to norepinephrine (NE) transporter (NET), dopamine (DA) transporter (DAT), and α2 receptor. Several of these enantiomers, (-)-I (R1 = R2 = H; R3 = 2-F), (-)-I (R1 = R2 = H; R3 = 3-F), (-)-I (R1 = H; R2 = 3-F; R3 = 2-F), (+)-I (R1 = H; R2 = R3 = 3-F), displayed a dual binding profile with affinities for SERT and NET with Ki < 25 nM and a NET/SERT ratio <10. (-)-I (R1 = R2 = H; R3 = 3-F) (coded as F-98214-TA for development studies) showed a dual binding profile with very high affinity values for SERT and NET (Ki = 1.9 and 13.5 nM, resp.), and further pharmacol. characterization is in progress for its evaluation as a antidepressant.

IT 639467-63-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of [(aryl)(aryloxy)alkyl]piperidines and analogs as potential antidepressants with high affinity for serotonin and norepinephrine transporters)

RN 639467-63-3 CAPLUS

CN Methanone, [1-[3-(2-fluorophenoxy)-3-phenylpropyl]-4-piperidinyl](4-fluorophenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> d his

     (FILE 'HOME' ENTERED AT 15:34:53 ON 30 JUN 2009)

     FILE 'REGISTRY' ENTERED AT 15:35:04 ON 30 JUN 2009
L1                STRUCTURE UPLOADED
L2             6 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 15:35:33 ON 30 JUN 2009
L3             2 S L2 FULL

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                      14.78     200.88

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                      -1.64      -1.64

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STRUCTURE FILE UPDATES:   29 JUN 2009  HIGHEST RN 1160357-19-6
DICTIONARY FILE UPDATES:  29 JUN 2009  HIGHEST RN 1160357-19-6

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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Uploading C:\Program Files\Stnexp\Queries\10594105last.str
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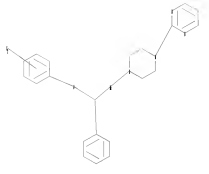

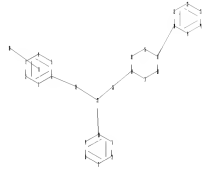

chain nodes :
25 26 27 30
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24
chain bonds :
6-25 10-27 14-26 17-20 25-27 26-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24
exact/norm bonds :
6-25 13-14 13-18 14-15 14-26 15-16 16-17 17-18 17-20 25-27 26-27
exact bonds :
10-27
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24
20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

G1:C,N

G2:CF2,CF3,CC12,CC13,CBr2,CBr3,X

G3:C,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 30:CLASS
31:Atom

L4 STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l4 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:39:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 283 TO ITERATE

100.0% PROCESSED 283 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

L5 6 SEA SSS FUL L4

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 185.88 386.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION
CA SUBSCRIBER PRICE 0.00 -1.64

FILE 'CAPLUS' ENTERED AT 15:39:57 ON 30 JUN 2009
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FILE COVERS 1907 - 30 Jun 2009 VOL 151 ISS 1
FILE LAST UPDATED: 29 Jun 2009 (20090629/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

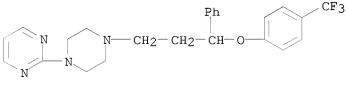
=> s l5 full
L6   7 L5

=> d ibib abs hitstr tot
THE ESTIMATED COST FOR THIS REQUEST IS 39.48 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L6 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2009:412461 CAPLUS
DOCUMENT NUMBER: 151:496
TITLE: QSAR study of the 5-HT1A receptor affinities of arylpiperazines using a genetic algorithm-artificial neural network model
AUTHOR(S): Habibi-Yangjeh, Aziz
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, University of Mohaghegh Ardabili, Ardabil, Iran
SOURCE: Monatshefte fuer Chemie (2009), 140(5), 523-530
CODEN: MOCMB7; ISSN: 0026-9247
PUBLISHER: SpringerWienNewYork
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Genetic algorithm-multiparameter linear regression (GA-MLR) and genetic algorithm-artificial neural network (GA-ANN) models have been used for prediction of the 5-HT1A receptor affinities (pK i) of 66 arylpiperazines. A large number of theor. descriptors were calculated for each compound The genetic algorithm (GA) was used for selection of the variables that resulted in the best fit to the MLR and ANN models. The models were generated using seven descriptors as variables. For evaluation of the predictive power of the models, pK i values of 13 compds. in the prediction set were calculated Mean percentage deviation (MPD) for the GA-MLR and GA-ANN models were 0.344 and 0.065, resp. Comparison of the results obtained by use of the models reveals the GA-ANN model is superior to the GA-MLR model. Graphical abstract

IT 328248-23-3
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR study of 5-HT1A receptor affinities of arylpiperazines using a genetic algorithm-artificial neural network model)
RN 328248-23-3 CAPLUS
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)

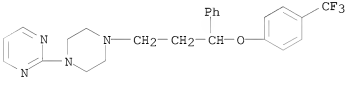


REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:803320 CAPLUS
DOCUMENT NUMBER: 149:215113
TITLE: Two-dimensional QSAR studies on arylpiperazines as high-affinity 5-HT1A receptor ligands
AUTHOR(S): Weber, Karen C.; Honorio, Kathia M.; Andricopulo, Adriano D.; Da Silva, Alberico B. F.
CORPORATE SOURCE: Instituto de Quimica de Sao Carlos, Universidade de Sao Paulo, Sao Carlos, 13560-970, Brazil
SOURCE: Medicinal Chemistry (2008), 4(4), 328-335
CODEN: MCEHAJ; ISSN: 1573-4064
PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 5-HT1A receptor plays an important role in the delayed onset of antidepressant action of a class of selective serotonin reuptake inhibitors. Moreover, 5-HT1A receptor levels have been shown to be altered in patients suffering from major depression. In this work, hologram quant. structure-activity relationship (HQSAR) studies were performed on a series of arylpiperazine compds. presenting affinity to the 5-HT1A receptor. The models were constructed with a training set of 70 compds. The most significant HQSAR model (q2 = 0.81, r2 = 0.96) was generated using atoms, bonds, connections, chirality, and donor and acceptor as fragment distinction, with fragment size of 6-9. Predictions for an external test set containing 20 compds. are in good agreement with exptl. results showing the robustness of the model. Addnl., useful information can be obtained from the 2D contribution maps.

IT 328248-23-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(two-dimensional QSAR studies on arylpiperazines as high-affinity 5-HT1A receptor ligands)
RN 328248-23-3 CAPLUS
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)



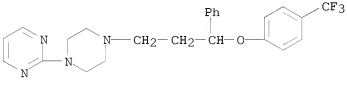
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:767635 CAPLUS
DOCUMENT NUMBER: 149:324283
TITLE: Quantitative structure-affinity relationship of 5-HT1A receptor ligands by the classification tree method
AUTHOR(S): Kuz'min, V. E.; Polischuk, P. G.; Artemenko, A. G.; Makan, S. Yu.; Andronati, S. A.
CORPORATE SOURCE: A.V. Bogatsky Physical-Chemical Institute, National Academy of Sciences of Ukraine, Odessa, Ukraine
SOURCE: SAR and QSAR in Environmental Research (2008), 19(3-4), 213-244
CODEN: SQERED; ISSN: 1062-936X
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The influence of mol. structure of 346 ligands on their affinity for 5-HT1A receptors was investigated. It was shown that the effectiveness of the proposed novel approach for interpretation of decision tree models compared favorably with the PLS method. In the context of the proposed approach, mol. fragments and their values of the relative influence on the affinity for 5-HT1A receptors were defined.

IT 328248-23-3
RL: ANT (Analyte); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study)
(quant. structure-affinity relationship of 5-HT1A receptor ligands by the classification tree method)

RN 328248-23-3 CAPLUS
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)



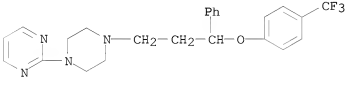
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:232006 CAPLUS
DOCUMENT NUMBER: 148:440268
TITLE: A chemometric study of the 5-HT1A receptor affinities presented by arylpiperazine compounds
AUTHOR(S): Weber, Karen C.; da Silva, Alberico B. F.
CORPORATE SOURCE: Instituto de Quimica de Sao Carlos, Universidade de Sao Paulo, Sao Carlos, 13566-590, Brazil
SOURCE: European Journal of Medicinal Chemistry (2008), 43(2), 364-372
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Elsevier Masson SAS
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Arylpiperazine compds. are promising 5-HT1A receptor ligands that can contribute for accelerating the onset of therapeutic effect of selective serotonin reuptake inhibitors. In the present work, the chemometric methods HCA, PCA, KNN, SIMCA and PLS were employed in order to obtain SAR and QSAR models relating the structures of arylpiperazine compds. to their 5-HT1A receptor affinities. A training set of 52 compds. was used to construct the models and the best ones were obtained with nine topol. descriptors. The classification and regression models were externally validated by means of predictions for a test set of 14 compds. and have presented good quality, as verified by the correctness of classifications, in the case of pattern recognition studies, and by the high correlation coeffs. (q^2 = 0.76, r^2 = 0.83) and small prediction errors for the PLS regression. Since the results are in good agreement with previous SAR studies, we can suggest that these findings can help in the search for 5-HT1A receptor ligands that are able to improve antidepressant treatment.

IT 328248-23-3
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(chemometric study of 5-HT1A receptor affinities presented by arylpiperazine compds. as possible antidepressants)

RN 328248-23-3 CAPLUS
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2006:847178 CAPLUS
DOCUMENT NUMBER: 145:410017
TITLE: Synthesis of benzenepropanamine analogues as non-detergent spermicides with antitrichomonas and anticandida activities
AUTHOR(S): Kumar, S. T. V. S. Kiran; Sharma, Vishnu Lal; Kumar, Manish; Shukla, Praveen Kumar; Tiwari, Pratibha; Jain, Rajeev Kumar; Maikhuri, Jagdamba Prasad; Singh, Divya; Gupta, Gopal; Singh, Man Mohan
CORPORATE SOURCE: Division of Medicinal and Process Chemistry, Central Drug Research Institute, Lucknow, 226001, India
SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(19), 6593-6600
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:410017
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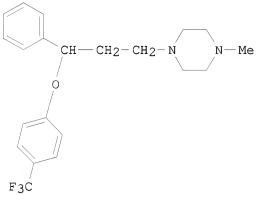


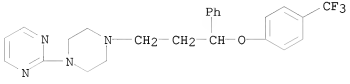
I

AB Fifteen analogs of benzenepropanamine were synthesized and evaluated for their spermicidal as well as microbicidal activities against Trichomonas vaginalis and Candida spp. Several compds. showed appreciable dual activities. Compound I exhibited good spermicidal (MEC = 0.1%) along with substantial anticandidal (MIC = 0.05%) activities, while compds. 3 and 6 showed significant microbicidal activities with moderate spermicidal effect. The SAR of these structures is being discussed here in this communication. It is concluded that suitable structural modifications in this class of compds. at 3-amino position may lead to a potent spermicide with associated microbicidal activity.
IT 911811-11-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(benzenepropanamine analogs as non-detergent spermicides with antitrichomonas and anticandida activities)

RN 911811-11-5 CAPLUS

CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]-, hydrochloride (1:2) (CA INDEX NAME)



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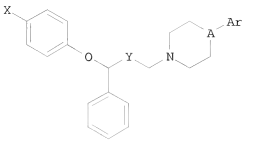
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:1103625 CAPLUS
DOCUMENT NUMBER: 143:387060
TITLE: Preparation of piperazine or piperidine derivatives as serotonin reuptake inhibitors
INVENTOR(S): Pinney, Kevin G.; Miranda, Maria Graciela; Dorsey, James Michael
PATENT ASSIGNEE(S): Baylor University, USA
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005094896	A2	20051013	WO 2005-US10356	20050328
WO 2005094896	A3	20070503		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AP, EA, EP, OA				
EP 1732610	A2	20061220	EP 2005-730778	20050328
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
US 20080132514	A1	20080605	US 2007-594105	20070921
PRIORITY APPLN. INFO.:			US 2004-557069P P	20040326
			WO 2005-US10356 W	20050328

OTHER SOURCE(S): CASREACT 143:387060; MARPAT 143:387060
GI



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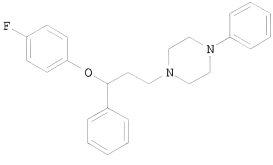


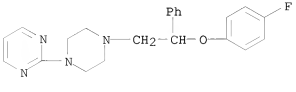
II

AB Title compds. I [X = F or CF3; Y = (CH2)n; n = 0-1; A = N or C; Ar = aryl] and their pharmaceutically acceptable salts, are prepared and disclosed as serotonin reuptake inhibitors. Thus, e.g., II was prepared by reduction of 1-phenyl-3-(4-phenyl-piperazin-1-yl)-propan-1-ol (preparation given) using sodium borohydride followed by coupling with 4-fluorophenol. The ability of I to inhibit [3H]5-HT uptake was evaluated using liquid scintillation spectroscopy and it was revealed that selected compds. of the invention possessed IC50 values in the range of 1.45 up to 9.56 μM. I as serotonin reuptake inhibitors should prove useful in the treatment of depression. Pharmaceutical composition comprising I are disclosed.

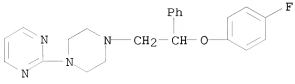
IT 866548-32-5P 866548-33-6P 866548-34-7P
866548-35-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperazine or piperidine derivs. as serotonin reuptake inhibitors)

RN 866548-32-5 CAPLUS

CN Pyrimidine, 2-[4-[2-(4-fluorophenoxy)-2-phenylethyl]-1-piperazinyl]- (CA INDEX NAME)



RN 866548-33-6 CAPLUS
CN Pyrimidine, 2-[4-[2-(4-fluorophenoxy)-2-phenylethyl]-1-piperazinyl]-, hydrochloride (1:1) (CA INDEX NAME)



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RN 866548-34-7 CAPLUS
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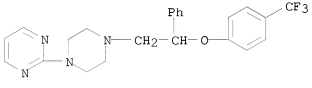
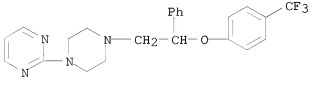


RN 866548-35-8 CAPLUS
CN Pyrimidine, 2-[4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-1-piperazinyl]-, hydrochloride (1:1) (CA INDEX NAME)



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L6 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:76 CAPLUS
DOCUMENT NUMBER: 134:207795
TITLE: New 1-aryl-3-(4-arylpiperazin-1-yl)propane derivatives, with dual action at 5-HT1A serotonin receptors and serotonin transporter, as a new class of antidepressants
AUTHOR(S): Martinez-Esparza, Javier; Oficialdegui, Ana-M.; Perez-Silanes, Silvia; Heras, Begona; Orus, Lara; Palop, Juan-A.; Lasheras, Berta; Roca, Joan; Mourelle, Marisa; Bosch, Ana; Del Castillo, Juan-C.; Tordera, Rosa; Del Rio, Joaquin; Monge, Antonio
CORPORATE SOURCE: Departments of Medicinal Chemistry and Pharmacology Centro de Investigacion en Farmacobiologia Aplicada (CIFA), Universidad de Navarra, Pamplona, 31080, Spain
SOURCE: Journal of Medicinal Chemistry (2001), 44(3), 418-428 CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:207795
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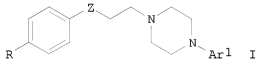

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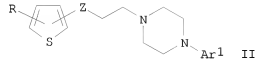

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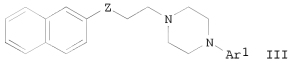
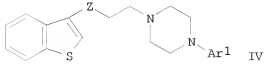


III



IV

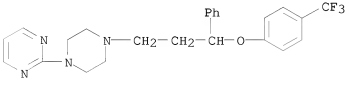
AB In a search toward new and efficient antidepressants, 1-aryl-3-(4-arylpiperazin-1-yl)propane derivs. I (R = H, Ph, MeO, NO2, Z = CO, CHOH, CHOR1, R1 = 4-F3CC6H4, 4-MeOC6H4, 3,4-OCH3OC6H3, Ar1 =

2-MeOC6H4, 4-ClC6H4, 2-pyridyl, etc.), II (R = H, 2,5-Me2, 5-Me, 5-NO2, Z = CO, CNOH, CHOH, CHOR1, R1 = 4-F3CC6H4, 3,4-OCH2OC6H3, 1-C10H7, position = 2, 3), III and IV (Ar1 = 2-MeOC6H4, 4-ClC6H4, 2-HOC6H4, Z = CO,CHOH) were designed, synthesized, and evaluated for 5-HT reuptake inhibition and 5-HT1A receptor antagonism. This dual pharmacol. profile should lead, in principle, to a rapid and pronounced enhancement in serotoninergic neurotransmission and consequently to a more efficacious treatment of depression. The design was based on coupling structural moieties related to inhibition of serotonin reuptake, such as γ-phenoxypropylamines, to arylpiperazines, typical 5-HT1A ligands. In binding studies, several compds. showed affinity at the 5-HT transporter and 5-HT1A receptors. Antidepressant-like activity was initially assayed in the forced swimming test with those compds. with Ki < 200 nM in both binding studies. Functional characterization was performed by measuring the intrinsic effect on rectal temperature in mice and also the antagonism to 8-OH-DPAT-induced hypothermia. The most efficacious compds. II (R = H, Z = CHO-1-C10H7, position = 3, Ar1 = 2-MeOC6H4) (V), II[R = 5-Me, Z = (E)-CNOH, position = 2, Ar1 = 2-MeOC6H4] and IV (Z = CO, CHOH, Ar1 = 2-MeOC6H4) (VI) were further explored for their ability to antagonize 8-OH-DPAT-induced inhibition of forskolin-stimulated cAMP formation in a cell line expressing the 5-HT1A receptor. Furthermore, the antidepressant-like properties of V and VI, which exhibited 5-HT1A receptor antagonistic property in the latter study, were also evaluated in the learned helplessness test in rats. Among these three compds., VI (Z = CHOH) (1-benzo[b]thiophene-3-yl)-3-[4-(2-methoxyphenyl)-1-ylpropan-1-ol] showed the higher affinity at both the 5-HT transporter and 5-HT1A receptors (Ki = 20 nM in both cases) and was also active in the other pharmacol. tests. Such a pharmacol. profile could lead to a new class of antidepressants with a dual mechanism of action and a faster onset of action.

IT 328248-23-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, 5-HT1A serotonin receptor antagonist and serotonin transporter activity, and structure-activity relationship of aryl(arylpiperazinyl)propanes)

RN 328248-23-3 CAPLUS

CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L2           6 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 15:35:33 ON 30 JUN 2009
L3           2 S L2 FULL

     FILE 'REGISTRY' ENTERED AT 15:39:28 ON 30 JUN 2009
L4             STRUCTURE UPLOADED
L5           6 S L4 FULL

     FILE 'CAPLUS' ENTERED AT 15:39:57 ON 30 JUN 2009
L6           7 S L5 FULL

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FULL ESTIMATED COST                                    39.98     426.74

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                    -5.74      -7.38

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